Meeting Enduring National Needs

As part of its overarching national security mission, the Department of Energy (DOE) pursues research and development in areas of enduring importance to the nation. DOE mission priorities in energy and environment, bioscience, fundamental science, and advanced technologies are supported by Laboratory research programs. Livermore seeks challenges that reinforce its national security mission and have the potential for high-payoff results.

Long-term research is essential to providing the nation with abundant, reliable energy as well as a clean environment. Livermore's energy and environmental programs contribute to the scientific and technological basis for secure, sustainable, and clean energy resources for the United States and to reducing risks to the environment.

Bioscience research at Livermore enhances the nation's health and security. Projects in genetics, molecular biology, computational biology, biotechnology, and health-care research leverage the Laboratory's physical science, computing, and engineering capabilities. Research is directed at understanding the causes of ill health, developing biodefense capabilities, improving disease prevention, and lowering health-care costs.

Leadership in science and engineering is also vital to the nation's long-term security. Many projects, sponsored by the DOE's Office of Science and other customers, take advantage of the unique research capabilities and facilities at Livermore. Other work, supported by Laboratory Directed Research and Development funding, aims at breakthroughs to extend the Laboratory's capabilities in anticipation of new mission requirements.

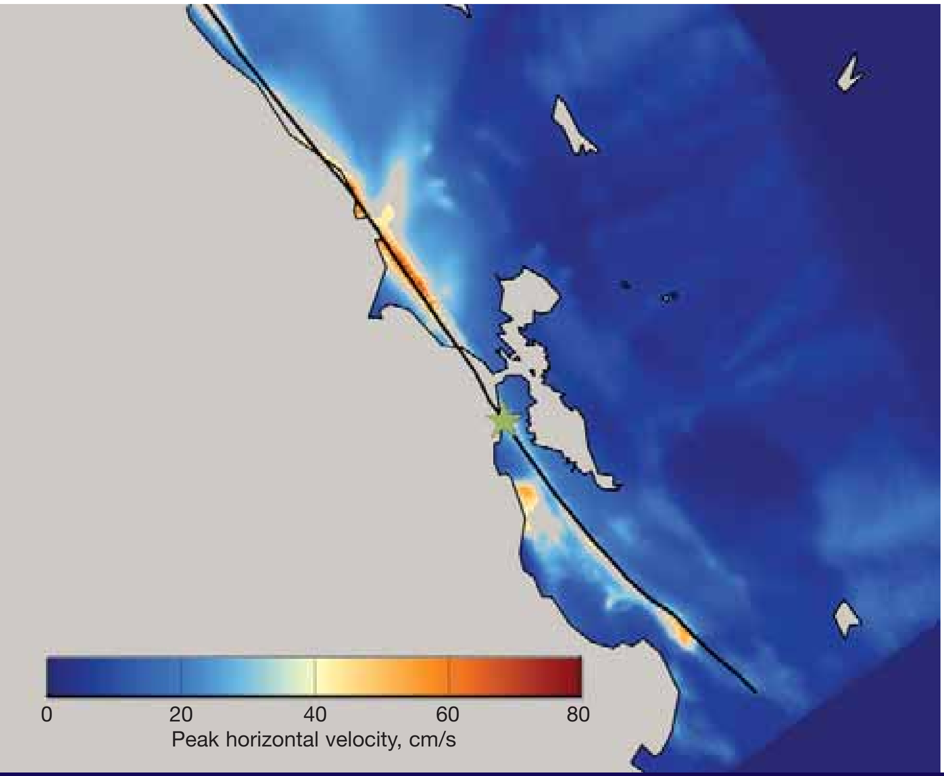
Scientific Discovery with Supercomputers

Ranked seventh on the Top500 List in June 2005, Livermore's Thunder supercomputer can process 23 trillion operations per second. It is available to Laboratory programs to run non-classified "grand challenge" problems—large calculations that promise breakthrough science. Since Thunder was installed in June 2004, researchers have used this Linux cluster for problems ranging in scale from high-resolution global and regional climate modeling to seismic simulations to protein folding and molecular dynamics.

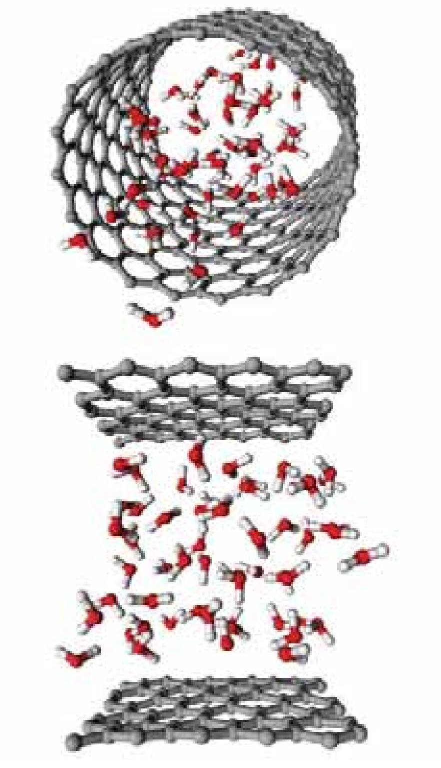
Because the properties of materials are important to almost all of the Laboratory's major programs, many grand challenge calculations are simulations of molecular dynamics. One important tool, named Qbox, uses the laws of quantum mechanics to describe the electrons in a system and then compute the interactions among atoms. Qbox makes possible predictions about material properties in cases where there are little data. Qbox on the Thunder machine can efficiently simulate hundreds of atoms for up to 20 picoseconds, allowing researchers to study nanotechnology, biochemistry, and high-energy-density physics. Qbox is also being optimized to run on the BlueGene/L supercomputer.

Researchers used Qbox to study the interaction between water and materials at the nanoscale. Their interest stems from plans to combine a nanoscale biological or chemical sensor with a nanofluidic device. Material properties change at the nanoscale, and subtle changes in a material's electronic and structural properties can be crucial to a device's performance. For example, simulations demonstrated that carbon tends to be hydrophobic, restricting the flow of water in carbon nanotubes or between closely spaced carbon graphite sheets. Results suggest that researchers may be able to prepare nanoscale materials with specific hydrophilic or hydrophobic properties.

Nanotubes are of particular interest for nanoscale electronic and mechanical applications because they are extremely



A simulation of the 1906 San Francisco earthquake is for a project with the U.S. Geological Service to better understand that quake and prepare for the next "Big One." For detailed simulations of the 1906 quake, see http://earthquake.usgs.gov/regional/nca/1906/simulations/.



Simulations of water molecules (red and white) confined within a carbon nanotube (top) and between carbon graphite sheets (above) demonstrate carbon's hydrophobic tendency.

strong and have good thermal conductivity. Researchers performed a series of quantum molecular dynamics simulations to examine the early growth of nanotubes, which must be carefully controlled for future applications. As reported in *Physical Review Letters*, the team studied different initial conditions of carbon covering nanoparticles of iron, which is a good catalyst for nanotube growth. They discovered that the carbon and iron do not mix at the nanoscale during growth and that the tubes grew capped.

New Supercomputing Tools

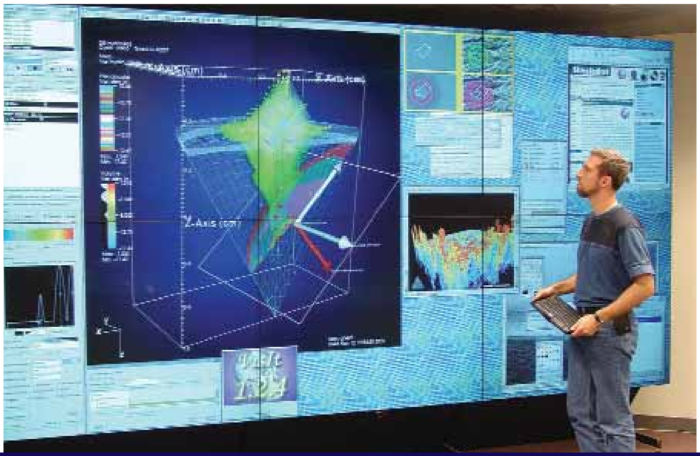
Scientific discovery through simulations requires more than codes optimized for highly parallel supercomputers; advanced tools for data management and visualization are needed as well. Laboratory users are benefiting from investments by the Advanced Simulation and Computing Program in new capabilities such as a powerful 256-node visualization cluster built by GraphStream Incorporated, which was delivered in September 2005. In addition, Livermore computer scientists are developing new knowledge extraction and visualization tools. One tool, dubbed VisIt, was an R&D100 Award winner in 2005 (see p. 49). Used to visualize data from a range of simulations codes, VisIt has a scalable architecture, allowing it to process some of the largest data sets ever generated.

Examining Materials Under Stress

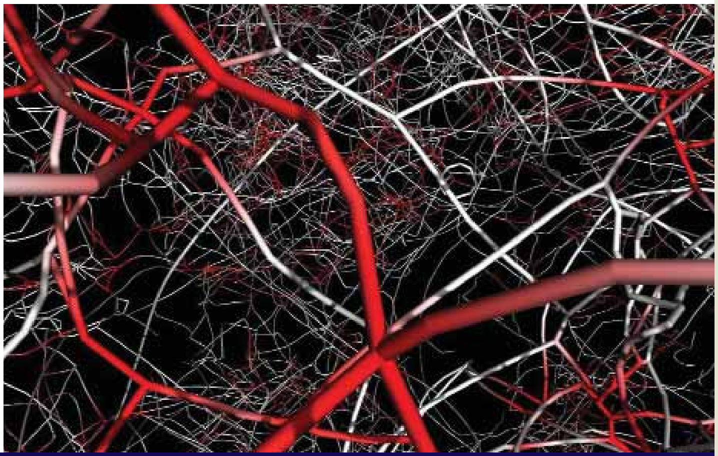
Experiments and advanced simulations are revealing further insights about material properties, especially in materials under stress. For wide-ranging applications, Livermore scientists need to understand what gives materials their strength and how and why they fail. Stockpile stewards, in particular, require detailed information about the properties of substances under extreme conditions.

In one set of activities, Laboratory scientists set out to better understand the mechanical properties of metals. The strength of most crystalline materials, including metals, derives from the motion, multiplication, and interactions of defects called dislocation lines. Simulations are providing unprecedented detail about dislocation dynamics—the interaction among dislocation lines. A new type of dislocation microstructure, known as a multijunction, was discovered through supercomputer simulations. The existence of multijunctions, which appear when three or more dislocations collide and form a knot, was confirmed in images taken with a transmission electron microscope. Multijunctions are thought to play an essential role in the strength evolution of crystalline metals as they deform.

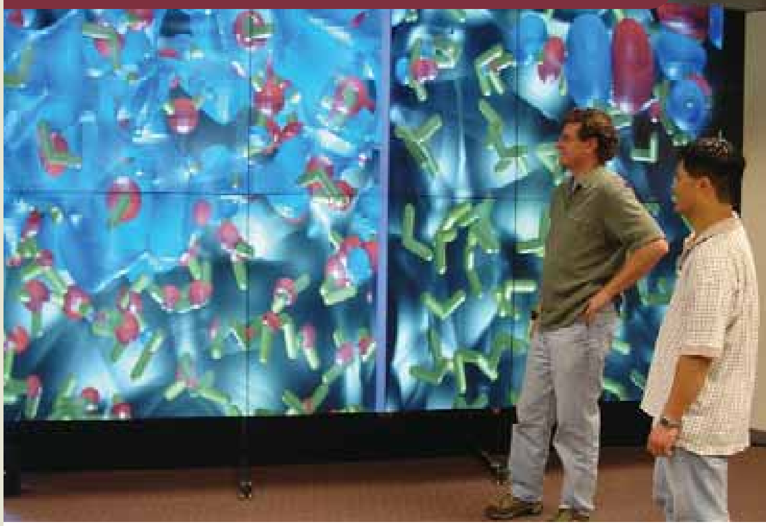
Other research performed by a Laboratory-led team and reported in *Science* points to the possibility of making superhard materials. Metallic materials are made of small "grains" joined by grain boundaries, which limit the movement of defects when the metal is stressed. Nanocrystalline materials, with grain size of less than 100 nanometers, are much harder than ordinary materials. However, when the



The VisIt visualization program, with a scalable architecture to study extremely large data sets, won an R&D 100 Award.



A new code, the Parallel Dislocation Simulator (ParaDiS), reveals new details about dislocation dynamics, including the source of strength hardening in stressed materials.



A quantum molecular dynamics simulation of water molecules.

grain size is reduced to tens of nanometers, deformations occur in a different way: the grains slide over each other. Using Livermore's Janus laser, researchers exposed nanocrystalline copper to an intense shock wave (about one-megabar pressure), which created additional defects within and between grains. These defects prevented the grains from sliding. The hardness of the material increased between 10 and 20 percent with each laser shot. Supercomputer simulations both confirmed and offered greater insight into the experimental results.

A very common substance—water—was studied under extreme conditions. As reported in *Physical Review Letters*, a team of Laboratory scientists created "superionic" water by squeezing a sample in a diamond anvil cell to a pressure of 470 kilobars and using a laser to heat it to 2400º F. Expected to be found inside giant planets like Neptune and Uranus, superionic water is neither ice nor liquid. The oxygen atoms are nearly stationary, while the hydrogen atoms are extraordinarily mobile. The researchers measured the frequency of the water molecules' vibrations and saw an abrupt change as the temperature rose, signaling a phase change. The observed optical spectra data were consistent with computer simulations of superionic water performed using Qbox and Thunder (see p. 24).

Interstellar Dust in the News

An exciting year in astrophysics at the Laboratory began and ended with dust in the news. In the January 14, 2005, issue of *Science*, Laboratory researchers and collaborators offered an explanation for a 40-year-old enigma in astronomy—why interstellar dust absorbs light at a wavelength of 2,175 angstroms. Using the latest transmission electron microscope and a nano-secondary ion mass spectrometer, the team analyzed interplanetary dust particles collected from the stratosphere by a high-flying NASA aircraft. Within the particles, they found the carriers of the 2,175-angstrom feature: organic carbon mixed with amorphous silicate grains about 100 nanometers in size, common materials in interstellar space. The measurements provide important clues about how interstellar matter was incorporated into the solar system.

A year later, on January 15, 2006, the Stardust spacecraft returned to Earth, having collected more pristine dust samples from interplanetary space and the tail of the Wild 2 comet. The

A Laboratory scientist gives the thumbs up upon learning that the Stardust spacecraft had successfully captured interplanetary dust and brought it back to Earth for study.

The very young stars in Minkowski's Object (central white globule) are being formed by the interaction of gas with a radio jet (in red) emanating from a nearby radio galaxy.

particles were captured in a grid filled with silica-based aerogel developed by Laboratory researchers, who also designed technologies to extract the samples from the aerogel. Livermore is part of the NASA-led team now analyzing the dust.

Using many of the same analysis techniques, Livermore scientists and collaborators also examined the oxygen and magnesium content of inclusions in a meteorite. As reported in *Nature*, these new data allowed the team to better estimate the lifetime of the solar nebula, the mass of dust and gas that eventually led to the formation of the solar system.

Stars and Galaxies Shine

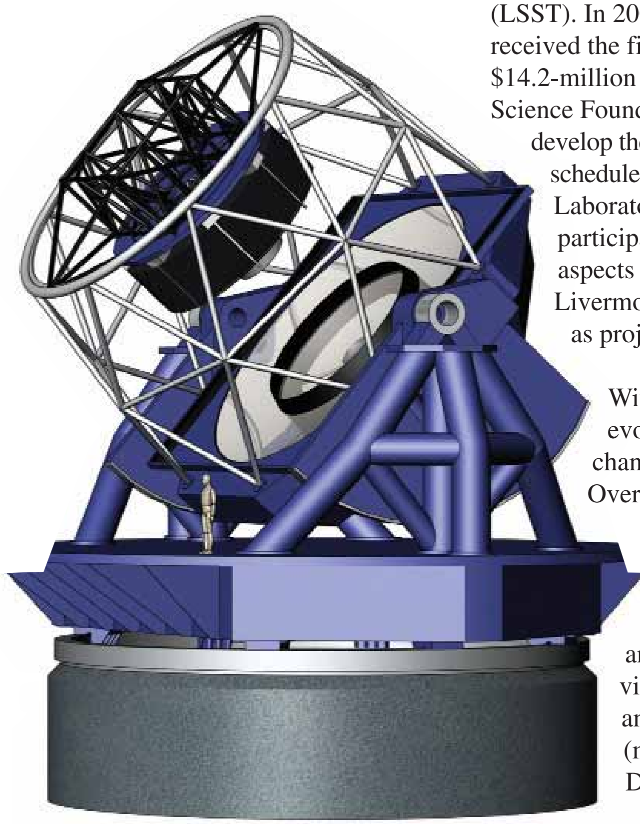
As reported in *Nature*, a Laboratory-led team has determined that stars form from the gravitational collapse of a gas cloud into massive clumps, which then evolve into stars. Through a series of supercomputer simulations, the team was able to rule out a competing theory, that the clumps are smaller and grow. Livermore's simulations show that turbulence in the gas cloud limits the rate at which clumps can accrete mass to become stars. Astronomers are observing too many stars in star-forming regions of the universe for the theory to be correct.

Laboratory researchers also combined computer simulations with optical and radio astronomy data to study and explain Minkowski's Object, a peculiar starburst system near the NGC 541 radio galaxy. In this system, perhaps 10 million stars are being created by a powerful jet of electrons, which is compressing warm, dense interstellar gas. The jet is emanating from the center of the radio galaxy where a black hole is accreting matter. This method of star formation is relatively rare today but may have been more common and significant in creating galaxies in the early universe. At that time, more hydrogen was available to create stars, and black holes were more active.

A New Window on the Universe

A very wide window for viewing the universe will open with construction of the Large Synoptic Survey Telescope (LSST). In 2005, the LSST project received the first part of a four-year, $14.2-million award from the National Science Foundation to design and develop the revolutionary telescope, scheduled for completion in 2012. Laboratory researchers are participating in virtually all aspects of the project, and a Livermore scientist is serving as project manager.

With its ability to record evolving events, LSST will change astronomy forever. Over a span of three nights, it will construct a complete, detailed map of the sky using a telescope with an 8.4-meter primary mirror, an extremely wide field of view (10-square-degrees), and an enormous camera (more than 3 billion pixels). Data from LSST's



The Large Synoptic Survey Telescope, which will map the entire sky every three nights, is expected to change astronomy forever.

astronomical surveys will be accessible almost immediately on the Web. When the telescope detects a changing object, such as an exploding supernova, it will send out an alert for more specialized telescopes to follow up with higher resolution images.

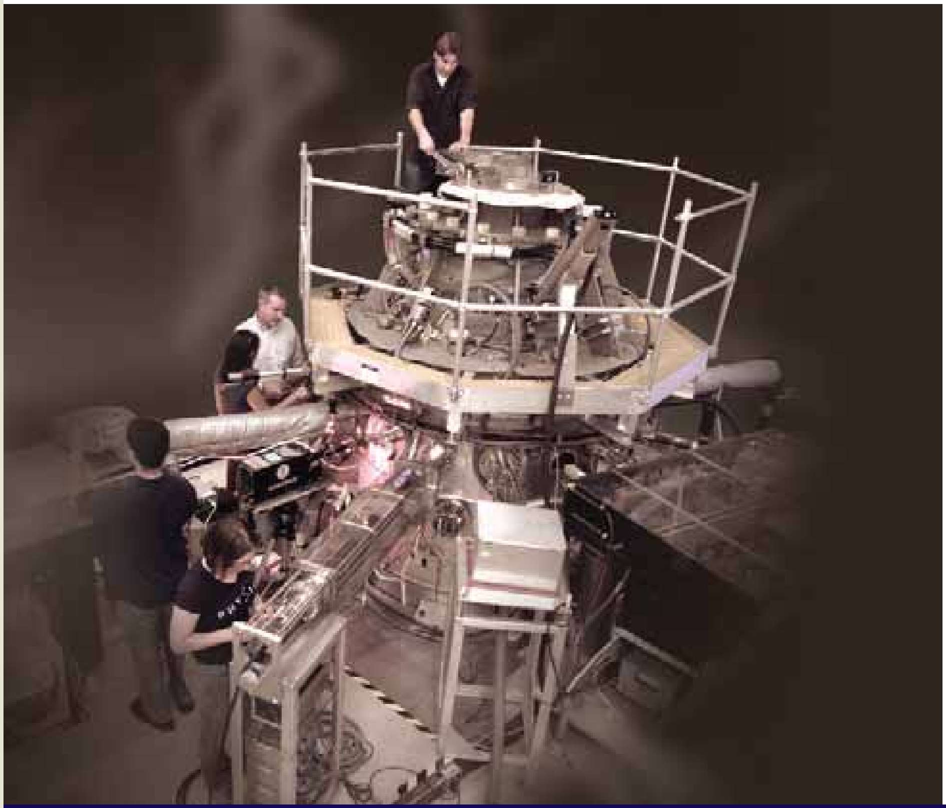
LSST will incorporate several technologies developed, for the most part, at the Laboratory. These include fabrication techniques for large optics developed for the recent generation of telescopes and the National Ignition Facility, the detector technologies for wide-angle cameras with billions of high-sensitivity pixels, and the technologies and tools for computing and storing large amounts of data (30 terabytes per night). Livermore helped pioneer wide-field-of-view, event-searching astronomy in the 1990s with the MACHO (Massively Compact Halo Object) project, which found evidence for one form of dark matter.

X-Ray Optics to Map the Sky

Livermore scientists are also engaged in programs to survey the sky in the hard x-ray (high-energy, greater than 20 keV) band of the spectrum. The Laboratory is part of a California Institute of Technology-led team proposing to build and launch a telescope named NuSTAR (Nuclear Spectroscopic Telescope Array), for which Livermore is contributing its special expertise in hard x-ray focusing optics. NuSTAR is part of NASA's Small Explorer Program, and a decision about proceeding to flight development is expected in early 2006.

NuSTAR's mission is to obtain a hard x-ray map of the sky in extraordinary resolution. Researchers intend to take a census of active black holes, which are powerful emitters of hard x rays, and they hope to measure the rate at which black holes are growing through the accretion of matter. Measurements of hard x rays from supernovae will also give scientists unprecedented information about physics deep inside exploding stars.

Laboratory scientists earlier worked with NuSTAR partners on the High Energy Focusing Telescope (HEFT), a balloon-launched hard x-ray telescope system. The Laboratory designed and fabricated the optics for the three telescopes and built the gondola. Launched on May 18, 2005, HEFT spent 20 hours nearly 40 kilometers above the Earth's surface, successfully imaging a dozen targets, including the Crab Nebula and the black hole Cygnus X-1. HEFT is providing the basis for the design and proposed production process for NuSTAR optics.



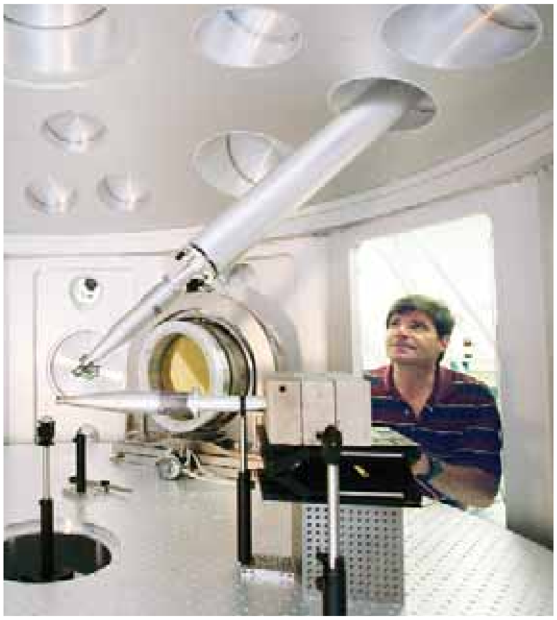
The "self-organizing" magnetized plasmas in the Sustained Spheromak Physics Experiment (SSPX) are similar to structures on the Sun and represent a possible route to fusion energy.

Fusion Energy Science Moves Ahead

The Laboratory is advancing fusion energy science through computational and experimental work performed for DOE's Office of Science. Livermore researchers are studying both the tokamak and spheromak approaches to magnetically confined fusion as well as inertial confinement fusion.

This year, an international agreement was signed to begin construction of the International Thermonuclear Experimental Reactor (ITER), a large tokamak designed to produce 500 megawatts of fusion power. The Laboratory has been participating in the ITER project since its inception. Livermore scientists working at the DIII-D Tokamak at General Atomics in San Diego have led the effort to develop new methods for reducing the heat load on the walls of ITER, and they are developing plasma diagnostics that the United States will install on ITER. In parallel, as part of DOE's Fusion Simulation Project, Livermore scientists are creating simulation tools to help understand how tokamak plasmas spontaneously form insulating surface layers. In these layers, plasma temperatures drop from more than 40 million degrees to a few thousand over a distance of just a few centimeters.

Livermore is examining an alternative to the tokamak concept at its Sustained Spheromak Physics Experiment (SSPX). The magnetized plasmas of a spheromak represent one possible route to commercial fusion energy, and the science of "self-organizing" magnetic dynamos is relevant to magnetic structures on the Sun and elsewhere. Research at the SSPX, which involves a large number of university collaborations, is aimed primarily at increasing the plasma's temperature and better understanding the role of turbulent magnetic fields in sustaining the plasma. Computer simulations at Livermore and Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center are contributing to the study of the spheromak's exceedingly complex plasma behavior.



Using the Titan laser, researchers can explore high-energy-density physics issues, including the science of fast ignition for inertial confinement fusion.

One of many areas of exploration for inertial confinement fusion (see p. 10) is the concept of fast ignition. First, a nanoseconds-long, high-energy laser pulse compresses a deuterium–tritium capsule. Then a high-intensity picoseconds-long laser pulse acts as a sparkplug to ignite the deuterium–tritium fuel. In October 2005, Livermore dedicated the Titan laser, the Laboratory's first combined long-pulse (nanosecond) and ultra-short-pulse (sub-picosecond) laser. Operating with hundreds of joules of energy in each beam, Titan is one of only three petawatt-class lasers in the world. Researchers will perform a range of high-energy-density physics experiments at Titan, including exploration of the science of fast ignition. The world's first petawatt (million-billion watt) laser was built at Livermore in the 1990s.

New Technologies for Storing Nuclear Waste

A team of Livermore researchers is testing and refining the design and materials for what eventually may be 12,000 nuclear waste packages as part of the DOE's program to design, license, and build an underground nuclear waste repository in Yucca Mountain, Nevada. The repository would house more than 70,000 metric tons of spent nuclear fuel from civilian nuclear power plants and highly radioactive waste from defense-related activities at DOE facilities across the United States.

Livermore has been the long-time lead for the advanced materials science of the waste packages. A new award-winning technique (see p. 50) offers a much improved way to characterize the aging of materials that protect the waste package. The technique allows researchers to better analyze the different phases of metal that form in accelerated-aging and elevated-temperature experiments, and to compare the results to predictions.

As part of a multi-institutional effort, Laboratory researchers are also developing high-performance, corrosion-resistant materials. New iron-based amorphous metals can be applied as coatings with advanced thermal spray technology to prevent exposure to environments that might cause stress cracking. Such materials could be used to coat the outer surface of waste containers for spent nuclear fuel or to protect welds and heat-affected zones.

Understanding Global Climate Change

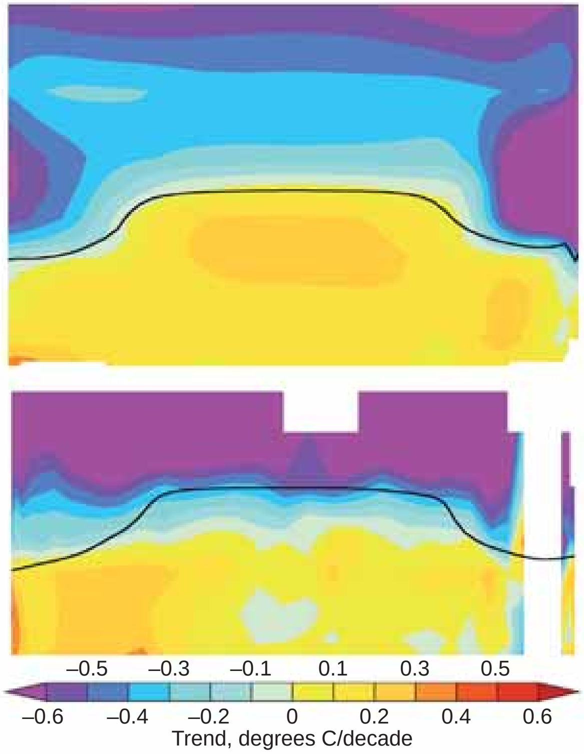
Three papers published in the August 11, 2005, edition of *Science Express* made an important contribution to the debate on global warming. The papers reconcile what had been a fundamental discrepancy between observed and modeled temperature trends in the tropical atmosphere. Until recently, climate modelers could compare their predictions of temperature increase with only one dataset, and those satellite observations showed a cooling of the tropical troposphere since 1979. The first two *Science Express* papers revisit temperature data obtained from satellites and weather balloons and provide compelling evidence that the tropical troposphere has warmed since 1979. The third study, led by a Laboratory scientist, finds that these new observational estimates of temperature change are consistent with the results from current climate models. Later in the year, that scientist, Benjamin Santer, was awarded a Distinguished Scientist Fellowship from the DOE Office of Science (see p. 48).

In another Laboratory-led study, researchers examined the consequences of humans continuing business as usual and using the entire planet's available fossil fuels by the year 2300. The polar ice caps will be depleted, ocean levels will rise by seven meters, and median air temperatures will soar to 8º C (14.5º F) warmer than today. The model predicts that the level of carbon dioxide in the atmosphere would rise from today's level of 380 parts per million (ppm) to more thsn 1,400 ppm by the year 2300. To the detriment of marine life, absorbed carbon dioxide would make the oceans more acidic. The results appeared in the *Journal of Climate*.

Managing Carbon

A variety of analyses, scientific studies, and technology development efforts at the Laboratory focus on the issues of carbon emissions and carbon management. To help energy futurists examine ways to reduce emissions, the Laboratory produces "U.S. Energy Flow Charts" each year and has done so for DOE since 1975. The charts, which are based on projections by the DOE's Energy Information Administration and other data sources, track energy supplies and demand. Data in the models also allow planners to study "carbon flow." Chart-making is now automated so that energy planners can study the implications of various what-if scenarios of energy supply, efficiency improvements, and demand.

A technique developed by two Laboratory scientists for reducing carbon dioxide emissions from power plants was patented in 2005. The process combines the carbon dioxide in power plant flue gas with water to produce a carbonic acid solution. The solution is mixed with limestone, which converts the acid to bicarbonate, and the bicarbonate is released into the ocean. Called carbonate weathering, the same geochemical reaction occurs in nature, only at a much slower pace. The process has less impact on marine life than the ongoing, passive uptake of excess carbon dioxide by



A Livermore-led team helped to reconcile the discrepancy between climate models (top) and weather balloon data (above) for temperatures in the tropical atmosphere.

the ocean or proposed injection of carbon dioxide into the deep sea.

A study published in *Nature* concludes that the Amazon basin is returning carbon to the atmosphere much faster than scientists had previously believed. Based on carbon-14 dating measurements at the Laboratory's Center for Accelerator Mass Spectrometry, the research team found that carbon being outgassed from Amazon waters has been stored in the surrounding landscape for only about five years. Previous measurements indicated that the age of carbon in the downstream sections of the Amazon basin was from 40 to more than 1,000 years.

Focus on the Genome

Biology has been playing a growing role in the Laboratory's interdisciplinary research in recent years, for which the emphasis on biodetection and biodefense (see p. 19) is partly responsible. In addition, since the completion of the Human Genome Project, Livermore continues to be a leader in genomic research.

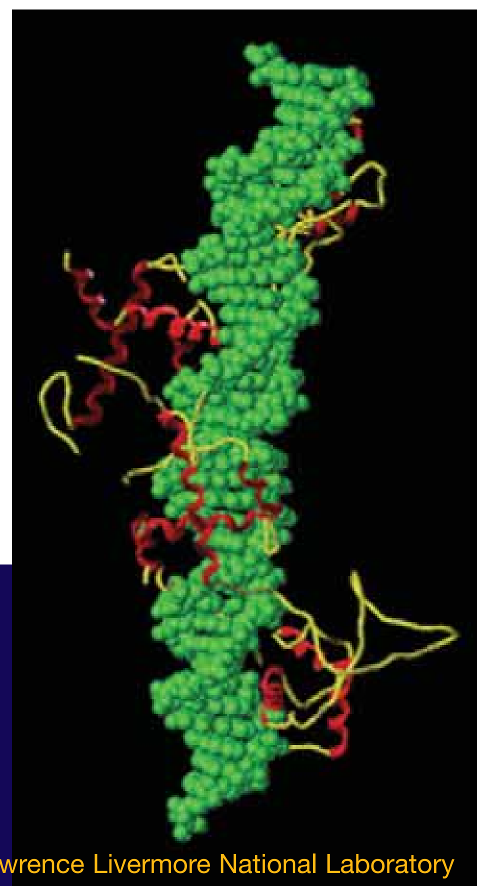
Laboratory scientists aim to determine the molecular functions of microbes that help regulate the planet's environment. One such study examined a community of microbes that thrives in hot, highly acidic conditions. Researchers from Lawrence Livermore and Oak Ridge national laboratories, the University of California at Berkeley, and Xavier University in New Orleans studied an Environmental Protection Agency Superfund site at an

Energy flow charts help visualize energy supply and demand, and their data allow planners to study "carbon flow."

abandoned mine at Iron Mountain, California. There they identified more than 2,000 proteins, more than 400 of which appear to be unique to this community. Their research, reported in *Science Express*, was the first to gather information on genes that are expressed within a natural community.

The field of comparative genomics is benefiting from work by a Livermore-led team of researchers. They developed analytical and visualization tools for identifying conserved DNA sequences, including gene regulatory elements that control gene expression and thereby play a major role in gene function and mechanisms of disease. These regulatory sequences are particularly enriched in "gene deserts," the large, mostly barren strings of DNA between genes. In one study, published in *Genome Research*, the researchers characterized especially large gene deserts that have persisted for hundreds of millions of years of evolution. Their new Web-based tools, which search all available sequenced genomes for regulatory elements, are now being used by medical and biological researchers worldwide as a resource for understanding genome function in many different species.

In another project related to gene expression, a team led by scientists from the Laboratory and Uppsala University in Sweden has developed a new bioinformatics technique for systematically analyzing key regions in DNA that help control gene activity. Binding sites, where DNA interacts with the proteins that control gene expression, can be far away from the genes they influence. Gene expression may also be controlled by several regulatory proteins (known as transcription factors) working



A new bioinformatics tool can locate sites where DNA interacts with proteins that control gene expression. Work started with much-studied yeast, including the yeast telomere-binding protein RAP1.

together at various binding sites. A machine-learning technique called rough sets mathematically modeled rules that associate known binding sites and gene expression in yeast, one of the most widely studied organisms. The team found that the same transcription factors, in slightly different combinations, could be responsible for the regulation of different genes. A large number of expression outcomes are possible using relatively few transcription factors.

Advanced Techniques Offer New Insight

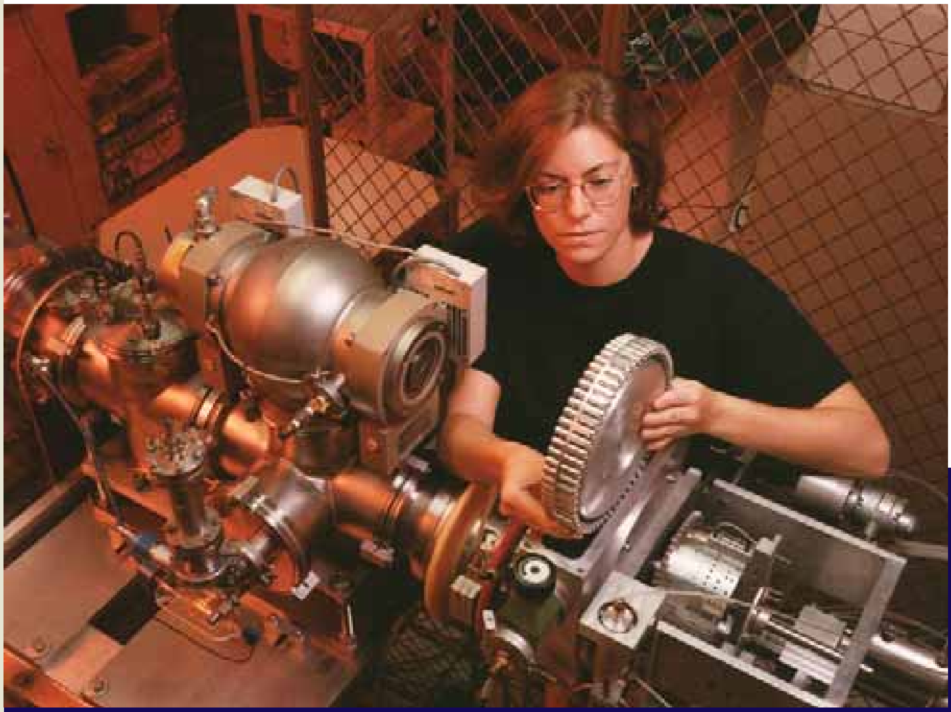
Well established experimental tools are being used in new ways to offer insight into important materials and natural processes. An example is the accelerator at the Center for Accelerator Mass Spectrometry, which is commonly used for carbon dating of archaeological and paleontological samples. In 2005, researchers used it to measure the age of DNA in human cells and tooth enamel. Swedish forensic scientists, who teamed with Livermore on the tooth enamel research, used enamel dating to help narrow the search for victims of the December 2004 tsunami in Southeast Asia.

Laboratory researchers combined breast cell-based assays with computational modeling and nuclear magnetic resonance (NMR) to better understand the link between the human diet and breast cancer. In this study, they examined a class of tumor-causing mutagens created when muscle meats such as beef, pork, and fowl are cooked. These mutagens, known by the acronym PhIP, may cause tumors in laboratory animals. The Livermore team developed methods that use NMR—most often used to determine the structure of proteins—to study whether molecules compete for the same binding location on a protein. NMR experiments confirmed simulation results that PhIP binds to the estrogen-receptor protein, activating estrogen receptors and stimulating breast cancer cells to proliferate. Understanding how diet affects the growth of hormone-sensitive cancers may eventually lead researchers to potent new therapeutics.

A Precise Measurement of a Basic Theory

Laboratory researchers tested quantum electrodynamics (QED)—an extension of quantum mechanics—to 10 times greater precision than any other recent measurements. The scientists entered a new realm in the search for QED deviations by measuring light generated in the extreme electric fields surrounding the nucleus of uranium. Deviations from QED would have far-reaching consequences for understanding the universe because they would indicate that QED is not in fact a fundamental theory of nature.

The team tested the theory using Livermore's SuperEBIT, an electron beam ion trap that strips atoms to a highly ionized state and holds the matter in place for hours while researchers study the emitted radiation. In the experiments, uranium atoms were stripped of all but three electrons, forming a uranium plasma. High-precision spectroscopy measurements allowed the team to extract an experimental value for the new QED effects, in which the polarized vacuum and the self-energy interacted with each other and themselves. Previous measurements only tested the noninteracting manifestations of QED. The team's results, which appeared in *Physical Review Letters*, will likely stimulate new experimental testing of QED predictions.



Discoveries at the Center for Accelerator Mass Spectrometry were cover news in three scientific journals in 2005.